High-End Computing

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Key Recommendations of the HECRTF Report

Overarching Goals

The HECRTF recommends that the Federal government and its private-sector partners carry out comprehensive,

HECRTF Plan's Proposed R&D Priorities to FY 2010

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This table provides an overview of the Federal HEC R&D

HEC I&A and R&D Programs By Agency

Selected FY 2004 Activities and FY 2005 Plans

High-end computing capabilities are important to work supported by all the NSF research directorates and offices including: Biological Sciences (BIO); Computer and Information Science and Engineering (CISE); Education and Human Resources (EHR); Engineering (ENG); Geosciences (GEO); Mathematical and Physical Sciences (MPS); and Social, Behavioral and Economic Sciences (SBE); and the Office of Polar Programs (OPP).

Directorates have complementary HEC investments. For example: R&D on computer architecture, networking, software, and cyberinfrastructure is funded by CISE; HEC devices are funded by MPS and ENG; mathematical algorithms are funded MPS and CISE; computational algorithms and libraries are funded by CISE, with some funding from MPS; science and engineering applications are developed primarily with funding from MPS, ENG, GEO,

cybertools (grid services and middleware, development tools, and libraries), domain-specific cybertools, and applications to make possible discovery and innovative education and training. The framework will consist of:

Council on Competitiveness HPC Initiative – HPCS-related co-funded by DARPA, DOE/SC, and

- Advanced data analysis and visualization technologies to explore and understand the vast amounts of data produced by this simulation

NASA HEC Resources

NASA high-end computing resources include:

- Goddard Space Flight Center, where the foci are in Earth Science and Space Science
  - 1,392 processing element (PE) Compaq (2.2 Teraflops)
  - 640 PE SGI O3K (410 Gigaflops)
  - Sun QFS (340 Terabytes)
  - SGI DMF (370 Terabytes)
- Ames, where the foci are in Aeronautics and Earth Science
  - 512 PE SGI Altix (2.3 teraflops)
  - 1,024 PE SGI O3K (850 gigaflops)
  - SGI DMF (1,600 terabytes)

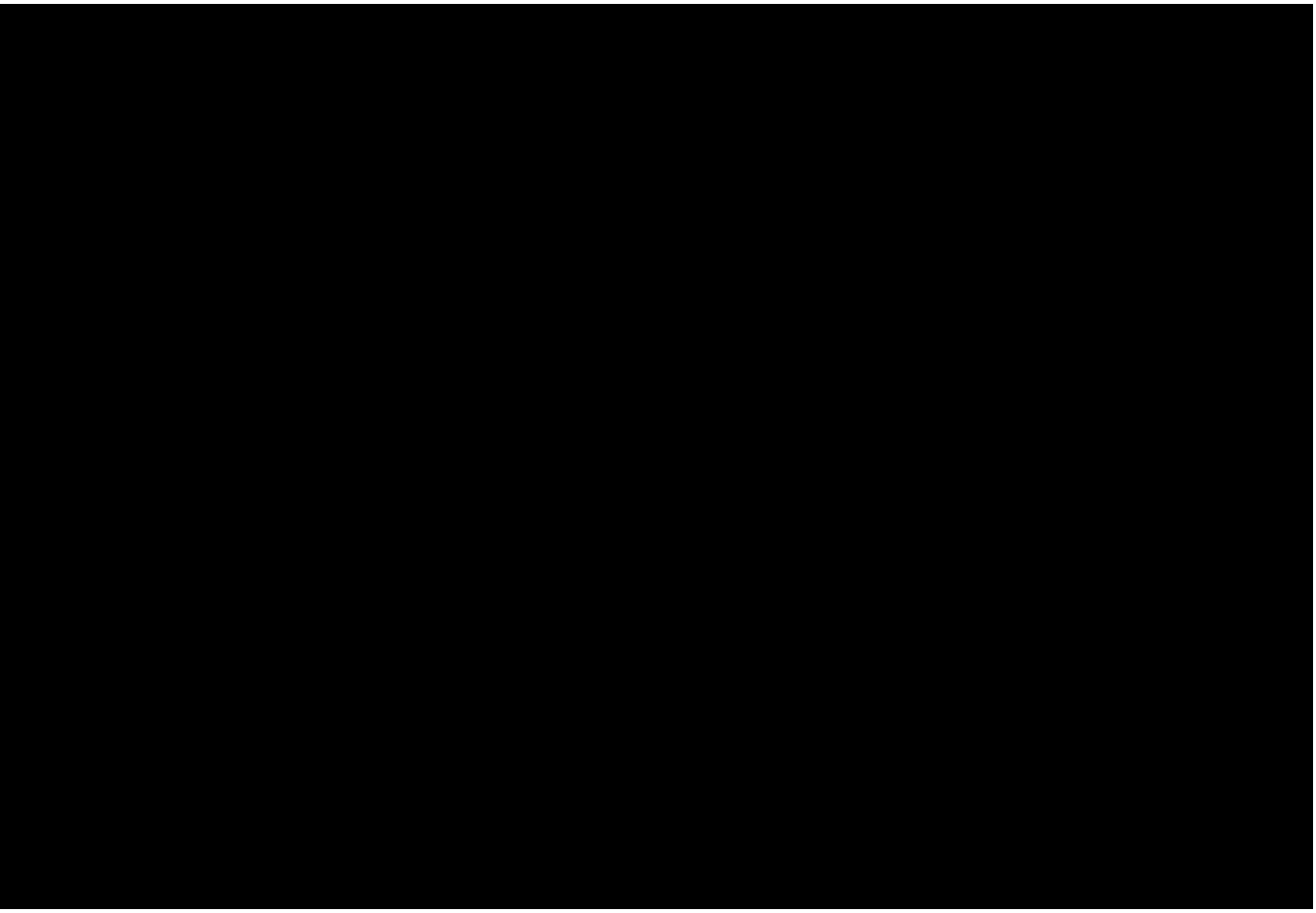
NASA FY 2005-FY 2007 HEC R&D plans include:

- *Collaborative decision systems to improve decision making*
- *Discovery systems to accelerate scientific progress*
- *Advanced networking and communncations*
- *Advanced computing architectures and technologies*
- *Reliable software*
- *Adaptive embedded information systems*

NSA has unclassified HEC R&D programs in the areas of:

- Architectures and systems
- High-speed switches and interconnects
- Programming environments
- Quantum information stiences
- Vendor partnerships

Cray X1e/Black Widow – under multiyear joint



EPA's mission is to protect human health and safeguard the environment through research, regulation, cooperation with state governments and industry, and enforcement. Areas of interest extend from groundwater to the stratosphere.

EPA HEC I&A programs are focused on tools to facilitate sound science using high-end computation, storage, and analysis. These programs enable relevant, high-quality, cutting-edge research in human health, ecology, pollution control and prevcemion, economics, and decision sciences. This facilitates appropriate characterization of scientific findings in the decision process. The HEC programs are performed in-house and as problem-drivce research.

EPA is launching the Center of Excellence (CoE– for Environmental Computational Science to integrate cutting-edge science and emerging IT solutions to facilitate Federal and state-level partnerships and enhance the availability of scientific tools and data for environmental decision making. The CoE will enable collaboration from within and without the organization and will provide a flexible, dynamic computing and information infrastructure to ensure optimized yet secure access to EPA resources.

FY 2004 HEC programs include:

Multimedia Assessments and Applications (MAA) Framework – provides a foundation for 0.0001 Tcon how to structure compartmental modules and improve model integration and interchangeability. The MAA framework's objectivc is to provide software that supports composing, configuring, applying, linking, and evaluating complex systems of object-oriented models. It will improve EPA's ability to simulate the interaction between individual environmental media components (e.g., chemical fluxes, water cycle– and will enable distributed computation.

The MAA framework is tailored to multimedia models but is adaptable and generalized. It supports EPA programs such as the Chesapeake Bay Program, the Tampa Bay Region Atmospheric Chemistry Experiment, and the Office of Air Quality Planning and Standards. The framework is currently being tested by a number of clients.

Uncertainty Analysis (UA) Framework Development – developing tools to support the analysis of media sensitivities and the effects of input uncertainties on media predictions. Specific tasks of this EPA work are to:

- Construct a 400-nedi Intel-based supercomputing cluster called SuperMUSE, for Supercomputer for Model Uncertainty and Sensitivity Evaluation
- Develop platform-independent systems software for managing SuperMUSE
- Conduct uncertainty and sensitivity analyses of the Multimedia, Multipathway, Multireceptor Risk Assessment (3MRA) mediaing system
- Develop advanced algorithmic software for advanced statistical sampaing methods and global sensitivity analyses

Air Quality Mediaing Applications (AQMA) – program aims to advance computational performance of the state-of-the-art Community Multiscale Air Quality (CMAQ) Chemistry-Transport Mediaing System while maintaining modularity, portability, and single-source code. Efforts to improve CMAQ take into account both the typical Linux cluster in the States and also HEC deployments. Major areas of effort include algorithmic improvement, microprocessor tuning, and 01 Titecture assessment. Involves a phased deployment that enables the states, whi Tcare the key stakeholders, to participate in the development.

Grid deployment – goal is to provide phased deployment of an EPA-wide enterprise grid ymentwill identify, develop, and integrate key technologies, align organizational policies such as security and networking, and field grid pilot systems to demonstrate success and benefits. Historically, agency 0.0001 Ters with high-end 0pplications competed for timecon EPA's high-performance computing resources located at the National Environmental Scientific Computing Center (NESC2). With the implementation of grid middleware, 0.0001 Ters will be able to tap unused processing capacity on local and remote clusters at the campus level or enterprise level. EPA's compute grid is being implemented in a phased 0pproach ic im1ateth the ty0bal rid 1j84e ty AQpute exheeenelopialign organizalyutsEPA-port ly, apment.

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Participating Agency

The mission of DoD's HPCMPO is to deliver world-class commercial, high-end, high-performance computational capability to DoD's science and technology (S&T) and test and evaluation (T&E) communities, thereby facilitating the rapid application of advanced technology in superior warfighting capabilities. Development of future technologies supported by HPC includes: Micro Air Vehicles; Joint Strike Fighter; surveillance systems; smart weapons design; ocean modeling; parachute simulations; Unmanned Air Vehicle; and blast protection.

HPCMPO requirements are categorized in the following ten key Computational Technology Areas (CTAs):

- Computational Structural Mechanics (CSM)
- Computational Fluid Dynamics (CFD)
- Computational Chemistry and Materials Science (CCM)
- Computational Electromagnetics and Acoustics (CEA)